



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3VX8 / pdb_00003vx8
Title : Crystal structure of Arabidopsis thaliana Atg7NTD-Atg3 complex
Authors : Matoba, K.; Fujioka, Y.; Noda, N.N.
Deposited on : 2012-09-11
Resolution : 3.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

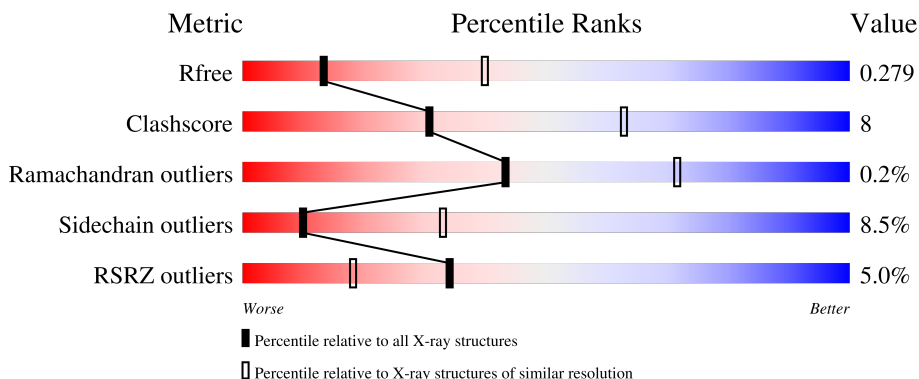
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	 2% (poor fit), 72% (0-1 outliers), 19% (2-3 outliers), 6% (not modelled)
1	D	323	 10% (poor fit), 71% (0-1 outliers), 18% (2-3 outliers), 7% (not modelled)
2	B	292	 % (poor fit), 46% (0-1 outliers), 12% (2-3 outliers), 40% (not modelled)
2	C	292	 2% (poor fit), 47% (0-1 outliers), 10% (2-3 outliers), 41% (not modelled)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquitin-like modifier-activating enzyme atg7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	300	Total	C	N	O	S	0	0	0
			2380	1533	396	444	7			
1	A	305	Total	C	N	O	S	0	0	0
			2418	1557	403	451	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	GLY	-	expression tag	UNP Q94CD5
D	4	PRO	-	expression tag	UNP Q94CD5
D	5	HIS	-	expression tag	UNP Q94CD5
D	6	MET	-	expression tag	UNP Q94CD5
A	3	GLY	-	expression tag	UNP Q94CD5
A	4	PRO	-	expression tag	UNP Q94CD5
A	5	HIS	-	expression tag	UNP Q94CD5
A	6	MET	-	expression tag	UNP Q94CD5

- Molecule 2 is a protein called Autophagy-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	Total	C	N	O	S	0	0	0
			1416	909	238	259	10			
2	C	172	Total	C	N	O	S	0	0	0
			1391	892	233	256	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	GLY	-	expression tag	UNP Q0WWQ1
B	23	PRO	-	expression tag	UNP Q0WWQ1
B	24	HIS	-	expression tag	UNP Q0WWQ1
B	25	MET	-	expression tag	UNP Q0WWQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	22	GLY	-	expression tag	UNP Q0WWQ1
C	23	PRO	-	expression tag	UNP Q0WWQ1
C	24	HIS	-	expression tag	UNP Q0WWQ1
C	25	MET	-	expression tag	UNP Q0WWQ1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.52Å 132.68Å 102.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.85 – 3.11 34.85 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.85-3.11) 99.1 (34.85-3.11)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.69 (at 3.12Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.278 0.226 , 0.279	Depositor DCC
R_{free} test set	1295 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtrriage
Anisotropy	0.076	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 16.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	4/2487 (0.2%)	0.87	6/3383 (0.2%)
1	D	0.52	1/2447 (0.0%)	0.81	2/3328 (0.1%)
2	B	0.38	0/1452	0.77	0/1966
2	C	0.38	0/1425	0.76	0/1929
All	All	0.54	5/7811 (0.1%)	0.82	8/10606 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	305	VAL	CA-CB	-7.00	1.50	1.55
1	A	307	TRP	CA-C	-6.45	1.45	1.52
1	A	307	TRP	NE1-CE2	-5.74	1.31	1.37
1	A	308	GLU	C-O	-5.32	1.17	1.23
1	A	229	HIS	CA-C	-5.03	1.47	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	GLY	N-CA-C	13.02	128.35	112.73
1	A	313	LYS	N-CA-C	5.86	118.61	109.52
1	A	303	ASN	N-CA-C	5.75	118.61	110.50
1	D	210	SER	N-CA-C	-5.69	98.68	110.80
1	A	39	ASP	CB-CA-C	-5.63	101.40	109.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	VAL	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2418	0	2358	50	0
1	D	2380	0	2323	45	0
2	B	1416	0	1412	18	0
2	C	1391	0	1386	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	7608	0	7479	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 125 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:SER:HB2	1:D:229:HIS:O	1.55	1.06
1:A:228:ASP:OD1	1:A:230:GLN:HB3	1.59	1.03
1:D:304:SER:O	1:D:305:VAL:HG23	1.65	0.97
2:B:193:ARG:HD2	2:B:222:LEU:HD11	1.51	0.92
1:D:209:SER:C	1:D:211:ASP:H	1.73	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/323 (93%)	284 (95%)	14 (5%)	1 (0%)	36	65
1	D	294/323 (91%)	275 (94%)	18 (6%)	1 (0%)	36	65
2	B	169/292 (58%)	164 (97%)	5 (3%)	0	100	100
2	C	166/292 (57%)	161 (97%)	5 (3%)	0	100	100
All	All	928/1230 (75%)	884 (95%)	42 (4%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ARG
1	D	306	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/286 (95%)	249 (92%)	22 (8%)	11	34
1	D	267/286 (93%)	244 (91%)	23 (9%)	10	32
2	B	160/259 (62%)	145 (91%)	15 (9%)	8	29
2	C	157/259 (61%)	144 (92%)	13 (8%)	10	34
All	All	855/1090 (78%)	782 (92%)	73 (8%)	10	33

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	279	GLU
2	C	268	ILE
2	B	304	MET
2	C	212	LEU
1	A	17	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	241	HIS
2	B	44	ASN
1	A	287	GLN
1	A	230	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/323 (94%)	-0.00	7 (2%) 61 39	18, 32, 56, 87	0
1	D	300/323 (92%)	0.79	32 (10%) 11 6	33, 56, 85, 108	0
2	B	175/292 (59%)	-0.02	3 (1%) 69 48	18, 33, 58, 89	0
2	C	172/292 (58%)	0.40	6 (3%) 47 27	33, 49, 74, 102	0
All	All	952/1230 (77%)	0.32	48 (5%) 34 18	18, 43, 79, 108	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	277	GLU	4.5
2	B	24	HIS	3.9
2	B	23	PRO	3.9
2	C	304	MET	3.6
1	D	182	ALA	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.